

# Spectrum of Coherent Modes for Trapped Bose Gas

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## Abstract

The spectrum of coherent modes for dilute atomic Bose gas, confined in a cylindrical trap, is calculated by applying optimized perturbation theory and the technique of self-similar root approximants. The latter technique makes it possible to derive accurate analytical formulas. The obtained expressions are valid for arbitrary energy levels of all excited nonlinear coherent modes and for different traps, spherical, sigar-shape, and disk-shape.

# 1 Introduction

At low temperatures, Bose-Einstein condensate of trapped atomic gases is well described by the Gross-Pitaevskii equation (see reviews [1–3]). In equilibrium, the condensate state corresponds to the ground-state solution of this equation. The mathematical structure of the Gross-Pitaevskii equation is identical to the nonlinear Schrödinger equation, which in the presence of a confining potential, should possess a discrete set of stationary states. Such states can be interpreted [4] as *nonlinear coherent modes* of trapped atoms [4] corresponding to *nonground-state Bose condensates*. The excitation of these modes can be accomplished by means of resonant modulation of an external potential [4–6]. Such modes have also been studied in Refs. [7–9] and a dipole mode has been observed experimentally [10].

One should not confuse the nonlinear coherent modes, that are stationary solutions to the *nonlinear* Gross-Pitaevskii equation, with elementary collective excitations, which are solutions of the *linear* Bogolubov-De Gennes equations. The nonlinear coherent modes are sometimes called *topological modes* to stress that their spatial behaviour qualitatively differs them from each other. Each nonlinear mode generates its own collective excitations as small deviations around the given mode. Usually, one considers collective excitations above the ground-state mode. These excitations correspond to small density fluctuations and are in a reasonable agreement with the Bogolubov spectrum for both superfluid helium [11] as well as for trapped Bose-Einstein condensate [12]. In the first case, it is the phonon-roton spectrum, which is a unified branch [13,14]. In the case of dilute trapped atoms, it is a phonon-single-particle branch. Collective excitations around nonground state coherent modes have not yet been considered.

Before considering perturbations of nonlinear coherent modes, it is necessary to have an accurate description of their own properties. In particular, one needs to better understand the features of the spectrum of the nonlinear modes themselves. The study of this spectrum was initiated in Ref. [4] and, for a weak interaction, was also considered in Ref. [9]. In the present paper, we aim at giving a general description of the nonlinear-mode spectrum for trapped atoms in a cylindrical trap. We shall describe a method for calculating arbitrary energy levels of this spectrum for any magnitude of the interaction parameter. We shall also construct accurate analytical expressions for the nonlinear-mode spectrum. Having in hands such analytical expressions is convenient for studying the spectrum dependence on quantum numbers and system parameters as well as for an easier comparison with experiments.

## 2 Equation for Coherent Modes

The interaction of atoms in dilute gases is characterized by the Fermi contact potential

$$\Phi(\mathbf{r}) = A\delta(\mathbf{r}) , \quad A \equiv 4\pi\hbar^2 \frac{a_s}{m_0} ,$$

in which  $a_s$  is the  $s$ -wave scattering length and  $m_0$ , the atomic mass. The trapping potential is usually taken in the form

$$U(\mathbf{r}) = \frac{m_0}{2} \left( \omega_x^2 r_x^2 + \omega_y^2 r_y^2 + \omega_z^2 r_z^2 \right) .$$

The stationary coherent field  $\varphi(\mathbf{r})$ , normalized to unity, is described [3] by the equation

$$\hat{H}[\varphi(\mathbf{r})]\varphi(\mathbf{r}) = E\varphi(\mathbf{r}) , \quad (1)$$

which is often called the Gross-Pitaevskii equation, with the nonlinear Hamiltonian

$$\hat{H}[\varphi(\mathbf{r})] = -\frac{\hbar^2 \nabla^2}{2m_0} + U(\mathbf{r}) + NA|\varphi(\mathbf{r})|^2 . \quad (2)$$

Because of the confining potential  $U(\mathbf{r})$ , the eigenproblem (1) possesses a discrete spectrum, with the related eigenfunctions being *nonlinear coherent modes* [4].

In what follows, we shall consider a harmonic potential of cylindrical symmetry, with a radial frequency

$$\omega_\perp \equiv \omega_x = \omega_y \quad (3)$$

and the anisotropy parameter

$$\nu \equiv \frac{\omega_z}{\omega_\perp} . \quad (4)$$

It is convenient to work with dimensionless quantities, measuring the space variables

$$r \equiv \frac{\sqrt{r_x^2 + r_y^2}}{l_\perp} , \quad z \equiv \frac{r_z}{l_\perp} \quad (5)$$

in units of the transverse oscillator length

$$l_\perp \equiv \sqrt{\frac{\hbar}{m_0 \omega_\perp}} . \quad (6)$$

The coupling parameter

$$g \equiv 4\pi \frac{a_s}{l_\perp} N \quad (7)$$

is a dimensionless quantity characterizing atomic interactions. Defining the dimensionless Hamiltonian and wave function, respectively,

$$\hat{H} \equiv \frac{\hat{H}[\varphi(\mathbf{r})]}{\hbar \omega_\perp} , \quad \psi(r, \varphi, z) \equiv l_\perp^{3/2} \varphi(\mathbf{r}) , \quad (8)$$

in the cylindrical coordinates, we have

$$\hat{H} = -\frac{1}{2} \nabla^2 + \frac{1}{2} (r^2 + \nu^2 z^2) + g|\psi|^2 , \quad (9)$$

where

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \varphi^2} + \frac{\partial^2}{\partial z^2} .$$

Then the eigenproblem (1) transforms to the equation

$$\hat{H}\psi_n = E_n\psi_n , \quad (10)$$

defining dimensionless coherent modes  $\psi_n$  and their spectrum  $\{E_n\}$ ;  $n$  being a multi-index labelling the modes. The latter are assumed to be normalized as

$$\int_0^\infty r \, dr \int_0^{2\pi} d\varphi \int_{-\infty}^{+\infty} dz |\psi_n(r, \varphi, z)|^2 = 1 .$$

Our aim is to find the spectrum  $\{E_n\}$  for all energy levels  $E_n$  of any quantum index  $n$  and for arbitrary coupling and anisotropy parameters  $g$  and  $\nu$ , respectively.

### 3 Optimized Perturbation Theory

To calculate the spectrum of the eigenproblem (10), we shall employ the optimized perturbation theory [15–19], which has been successfully applied to a number of models in quantum mechanics, statistical physics, and quantum field theory [15–26]. Numerous references on various applications can be found in surveys [27–29]. It is important to stress that the optimized perturbation theory was shown to provide accurate results for all energy levels and large coupling parameters.

For the case considered, the procedure can be as follows. We start with the initial Hamiltonian of a harmonic oscillator

$$\hat{H}_0 = -\frac{1}{2} \nabla^2 + \frac{1}{2} (u^2 r^2 + v^2 z^2) , \quad (11)$$

having the oscillator strengths as two trial parameters,  $u$  and  $v$ . This Hamiltonian possesses the eigenvalues

$$E_{nmj}^{(0)} = (2n + |m| + 1)u + \left(j + \frac{1}{2}\right)v , \quad (12)$$

with the radial quantum number  $n = 0, 1, 2, \dots$ , azimuthal number  $m = 0, \pm 1, \pm 2, \dots$ , and the axial quantum number  $j = 0, 1, 2, \dots$ . The corresponding wave functions are

$$\begin{aligned} \psi_{nmj}^{(0)}(r, \varphi, z) &= \left[ \frac{2n! u^{|m|+1}}{(n + |m|)!} \right]^{1/2} r^{|m|} \exp\left(-\frac{u}{2} r^2\right) \times \\ &\times L_n^{|m|}(ur^2) \frac{e^{im\varphi}}{\sqrt{2\pi}} \left(\frac{v}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^j j!}} \exp\left(-\frac{v}{2} z^2\right) H_j(\sqrt{v} z) , \end{aligned} \quad (13)$$

where  $L_n^m(\cdot)$  is a Laguerre polynomial and  $H_j(\cdot)$  is a Hermite polynomial.

Using a variant of the standard perturbation theory, such as the Rayleigh-Schrödinger theory, we may find a sequence  $\{E_k(g, u, v)\}$  of the energies  $E_k(g, u, v)$  for the approximation orders  $k = 0, 1, 2, \dots$ . Here, for the simplicity of notation, the dependence of the energy levels on the quantum numbers is not written down explicitly, but it is assumed. For instance,  $E_0(g, u, v) = E_{nmj}^{(0)}$ . Then the trial parameters are to be transformed to control functions [15–19]  $u_k(g)$  and  $v_k(g)$  such that to render the sequence  $\{e_k(g)\}$  of the *optimized terms*

$$e_k(g) \equiv E_k(g, u_k(g), v_k(g)) \quad (14)$$

convergent. The control functions can be found from optimization conditions. For example, we may employ the fixed-point condition

$$\left( \delta u \frac{\partial}{\partial u} + \delta v \frac{\partial}{\partial v} \right) E_k(g, u, v) = 0 , \quad (15)$$

whose solutions are  $u = u_k(g)$  and  $v = v_k(g)$ . The *optimized approximants* (14) are valid for arbitrary quantum numbers and for the whole range of the coupling parameter  $g$ . The same procedure can be used for anharmonic traps, described by anharmonic confining potentials of different powers [29], integer or noninteger. Note that the usage of anharmonic traps may be important for some experiments [30] dealing with elementary collective excitations.

In the first order, we have the energy

$$E_1(g, u, v) = \frac{p}{2} \left( u + \frac{1}{u} \right) + \frac{q}{4} \left( v + \frac{\nu^2}{v} \right) + u\sqrt{v} g I_{nmj} , \quad (16)$$

in which the notation

$$p \equiv 2n + |m| + 1 , \quad q \equiv 2j + 1 \quad (17)$$

for the combinations of quantum numbers is introduced and where

$$\begin{aligned} I_{nmj} &\equiv \frac{1}{u\sqrt{v}} \int |\psi_{nmj}^{(0)}(r, \varphi, z)|^4 r dr d\varphi dz = \\ &= \frac{2}{\pi^2} \left[ \frac{n!}{(n + |m|)! 2^j j!} \right]^2 \int_0^\infty x^{2|m|} e^{-2x} [L_n^{|m|}(x)]^4 dx \int_0^\infty e^{-2t^2} H_j^4(t) dt . \end{aligned}$$

The fixed-point condition (15) gives the equations

$$p \left( 1 - \frac{1}{u^2} \right) + \frac{s}{p\nu} \sqrt{\frac{v}{q}} = 0 , \quad q \left( 1 - \frac{\nu^2}{v^2} \right) + \frac{us}{p\nu\sqrt{vq}} = 0 \quad (18)$$

for the control functions  $u = u_1(g)$  and  $v = v_1(g)$ , where, for convenience, the notation

$$s \equiv 2p\sqrt{q} g \nu I_{nmj} \quad (19)$$

is used. Substituting the solutions for the control functions, given by Eqs. (18), in the form (16) results in the optimized approximant  $e_1(g)$ , according to definition (14). This

procedure can be continued to a desired approximation order. Here we limit ourselves by the first-order approximation

$$E \equiv e_1(g) = E_1(g, u_1(g), v_1(g)) , \quad (20)$$

in which the control functions  $u_1(g)$  and  $v_1(g)$  are the solutions of Eqs. (18). The latter equations, for a given set  $\{n, m, j\}$  of quantum numbers and a coupling parameter  $g$ , require a numerical solution. Hence, the spectrum (20) can be calculated only numerically. However, it is always desirable to possess an approximate analytical expression that could be easy to treat with respect to varying system parameters, such as quantum numbers and the coupling parameter.

## 4 Self-Similar Root Approximants

In order to derive analytical formulas for the spectrum of the nonlinear coherent modes, we may employ the technique of self-similar crossover approximants [31,32]. For this purpose, we need to know the asymptotic expansions of the spectrum in the limits of the weak and strong coupling. These expansions for the spectrum (20) can be derived from Eqs. (16) and (18). It is convenient to use the variable (19) that is proportional to the coupling parameter; so that if  $g \rightarrow 0$ , then  $s \rightarrow 0$ , and when  $g \rightarrow \infty$ , then  $s \rightarrow \infty$ . In the weak-coupling limit, we find the expansion

$$E \simeq a_0 + a_1 s + a_2 s^2 + a_3 s^3 , \quad (21)$$

as  $s \rightarrow 0$ , where

$$a_0 = p + \frac{q\nu}{2} , \quad a_1 = \frac{1}{2p(q\nu)^{1/2}} , \quad a_2 = -\frac{p + 2q\nu}{16p^3(q\nu)^2} , \quad a_3 = \frac{(p + 2q\nu)^2}{64p^5(q\nu)^{7/2}} .$$

In the strong-coupling limit, we obtain

$$E \simeq b_0 s^{2/5} + b_1 s^{-2/5} + b_2 s^{-6/5} + b_3 s^{-2} + b_4 s^{-14/5} + b_5 s^{-18/5} , \quad (22)$$

as  $s \rightarrow \infty$ , where

$$\begin{aligned} 4b_0 &= 5 , & 4b_1 &= 2p^2 + (q\nu)^2 , & 20b_2 &= -3p^4 + 2p^2(q\nu)^2 - 2(q\nu)^4 , \\ 20b_3 &= 2p^6 - p^4(q\nu)^2 - 2p^2(q\nu)^4 + 2(q\nu)^6 , \\ 500b_4 &= -44p^8 + 22p^6(q\nu)^2 + 2p^4(q\nu)^4 + 78p^2(q\nu)^6 - 69(q\nu)^8 , \\ 12500b_5 &= 1122p^{10} - 595p^8(q\nu)^2 - 70p^6(q\nu)^4 + 440p^4(q\nu)^6 - 3640p^2(q\nu)^8 + 2821(q\nu)^{10} . \end{aligned}$$

The asymptotic expansions (21) and (22), valid in the weak-coupling limit  $s \rightarrow 0$  and, respectively, in the strong-coupling limit  $s \rightarrow \infty$ , can be sewed by using the technique of self-similar crossover approximants [31,32]. This technique makes it possible to construct interpolative formulas that provide correct asymptotic expansions, at the same time giving

good accuracy in the whole interval of the variable  $s$ . The detailed description of the method can be found in Refs. [31,32]. Taking into account only one term in the strong-coupling expansion (22), we get the first-order self-similar root approximant

$$E_1^* = a_0(1 + As)^{2/5}, \quad (23)$$

in which

$$a_0 = p + \frac{q\nu}{2}, \quad Aa_0^{5/2} = 1.746928.$$

Retaining two terms in Eq. (22) yields the second-order approximant

$$E_2^* = a_0 \left[ (1 + A_1 s)^{6/5} + A_2 s^2 \right]^{1/5}, \quad (24)$$

where  $a_0$  is the same as in Eq. (23) and

$$A_1 a_0^{25/6} = 2.533913 \left[ 2p^2 + (q\nu)^2 \right]^{5/6}, \quad A_2 a_0^5 = 3.051758.$$

Similarly, in the third order we find

$$E_3^* = a_0 \left\{ \left[ (1 + B_1 s)^{6/5} + B_2 s^2 \right]^{11/10} + B_3 s^3 \right\}^{2/15}, \quad (25)$$

where  $a_0$  is again as earlier and

$$B_1 a_0^{125/22} \left[ 2p^2 + (q\nu)^2 \right]^{5/66} = 1.405455 \left[ 8p^4 + 12p^2(q\nu)^2 + (q\nu)^4 \right]^{5/6},$$

$$B_2 a_0^{75/11} \left[ 2p^2 + (q\nu)^2 \right]^{10/11}, \quad B_3 a_0^{15/2} = 5.331202.$$

In the same way, we may construct higher-order approximants, which, however, we will not write down explicitly.

Let us stress that the self-similar root approximants (23) to (25) are valid for the whole range of variable (19), related to the coupling parameter (7); they are also valid for an arbitrary anisotropy parameter (4), incorporated in the variable (19), as well as for all quantum numbers that enter expressions (23) to (25) through the parameters (17) and the variable (19). The accuracy of the root approximants can be checked by comparing their values with those obtained numerically from Eqs. (18) and (20).

Bose-Einstein condensates are often treated by using the Thomas-Fermi approximation, when one omits the kinetic energy operator in Eq. (10). In such a case, the solution to Eq. (10) reads

$$\psi_{TF}(r, z) = \Theta \left( r_0^2 - r^2 - \nu^2 z^2 \right) \left( \frac{r_0^2 - r^2 - \nu^2 z^2}{2g} \right)^{1/2},$$

where  $r_0^2 \equiv 2E_{TF}$  and the energy is obtained from the normalization condition for  $\psi_{TF}$ , which results in the expression

$$E_{TF} = \frac{1}{2} \left( \frac{15}{4\pi} g\nu \right)^{2/5}.$$

The Thomas-Fermi approximation is not self-consistent since the average of the Hamiltonian (9), calculated with the wave function  $\psi_{TF}$ , diverges. The energy  $E_{TF}$  becomes correct for an asymptotically large coupling parameter  $g \rightarrow \infty$ , but for small and intermediate  $g$  this formula is not accurate. There have been several suggestions of improving the Thomas-Fermi approximation by means of additional corrections [33–35]. However, even after being improved, this approximation provides us solely the ground-state energy, being unable to describe the excited energy levels of the nonlinear coherent modes.

Figure 1 shows the ground-state energy of the condensate in a cigar-shape trap, with  $\nu = 0.1$ , calculated in different approximations. For comparison, the Thomas-Fermi energy is also presented although its accuracy up to the coupling parameters  $g \approx 300$  is quite bad. The maximal errors for the self-similar root approximants from  $E_1^*$  to  $E_5^*$  are, respectively: 8%, 3.5%, 2%, 1.2%, and 0.8%, which demonstrates good convergence.

The accuracy of the self-similar root approximants for different energy levels of the coherent modes, varying the coupling parameter  $g$ , and for different trap shapes is illustrated in Figures 2 to 4, where the percentage errors as functions of  $g$  are drawn for a cigar-shape trap (Fig. 2), spherical trap (Fig.3), and a disk-shape trap (Fig.4). In all cases, there is the following standard situation. The maximal, with respect to  $g$  and quantum numbers, percentage errors for  $E_1^*$  are between 4–12%; for  $E_2^*$ , between 2–5%, and for  $E_3^*$ , of order 1%. The approximants  $E_4^*$  and  $E_5^*$  are close to  $E_3^*$ , because of which, not to overload the Figures, they are often omitted.

## 5 Conclusion

The nonlinear coherent modes of Bose-Einstein condensate at zero temperature are studied. These are described by the Gross-Pitaevskii equation and correspond to the stationary solutions of the latter. In the presence of a trapping potential, the spectrum of the coherent modes is discrete. Our main aim in this paper was to find a convenient and accurate way of calculating the energy levels of this spectrum for arbitrary quantum numbers, any values of coupling parameters, and for different aspect ratios of a cylindrical trap. One way for calculating the spectrum is by employing optimized perturbation theory, which requires numerical solution of the equations for control functions. Another possibility is to invoke the technique of self-similar root approximants, which results in sufficiently simple, and at the same time accurate, analytical formulas for the spectrum. The advantage of possessing analytical expressions is in the feasibility of a relatively easy study of their behaviour with respect to all parameters characterizing the system. And to understand better the properties of the coherent modes is necessary for choosing the optimal conditions for their experimental observation and practical usage.

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## Figure Captions

**Fig. 1.** The ground-state energy for a cigar-shape trap, with  $\nu = 0.1$ , as a function of the coupling parameter  $g$ , calculated by using formula (20) (solid line), and the self-similar root approximants  $E_1^*$  (long-dashed line),  $E_2^*$  (short-dashed line), and  $E_3^*$  (dotted line). The energy  $E_{TF}$  in the Thomas-Fermi approximation is shown by the dashed-dotted line.

**Fig. 2.** The percentage errors of the self-similar root approximants for the energy levels of coherent modes in a cigar-shape trap, with  $\nu = 0.1$ , corresponding to  $E_1^*$  (solid line),  $E_2^*$  (long-dashed line),  $E_3^*$  (short-dashed line),  $E_4^*$  (dotted line), and  $E_5^*$  (dashed-dotted line) for different quantum numbers: (a)  $n = m = j = 0$ ; (b)  $n = j = 0$ ,  $m = 2$ ; (c)  $n = j = 0$ ,  $m = 10$ .

**Fig. 3.** Percentage errors of the self-similar root approximants for  $E_1^*$  (solid line),  $E_2^*$  (long-dashed line), and  $E_3^*$  (short-dashed line) for a spherical trap, with  $\nu = 1$ , and for different energy levels: (a)  $n = m = j = 0$ ; (b)  $n = j = 0$ ,  $m = 2$ ; (c)  $n = 3$ ,  $m = 2$ ,  $j = 1$ .

**Fig. 4.** The case of a disk-shape trap with  $\nu = 10$ . Percentage errors of the approximants  $E_1^*$  (solid line),  $E_2^*$  (long-dashed line),  $E_3^*$  (short-dashed line) and  $E_4^*$  (dotted line) for different coherent modes: (a)  $n = m = j = 0$ ; (b)  $n = j = 0$ ,  $m = 2$ ; (c)  $n = 3$ ,  $m = 2$ ,  $j = 1$ .